# Full $0\hbar\omega$ shell model calculation of the binding energies of the $1f_{\frac{7}{2}}$ nuclei

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Binding energies and other global properties of nuclei in the middle of the $pf$ shell, such as M1, E2 and Gamow-Teller sum rules, have been obtained using a new Shell Model code (NATHAN) written in quasi-spin formalism and using a $j$-$j$-coupled basis. An extensive comparison is made with the recently available Shell Model Monte Carlo results using the effective interaction KB3. The binding energies for -nearly- all the $1f_{7/2}$ nuclei are compared with the measured (and extrapolated) results.

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## I. INTRODUCTION

Detailed Shell Model calculations in the full $pf$-shell have been recently carried out [1–3] up to $A = 52$ using a realistic G-matrix [4] with the monopole modifications of ref. [5] (KB3). These calculations could only be done due to the availability of the $m$-scheme code ANTOINE [6]. It has allowed us to tackle the largest dimensionalities ever reached by any exact diagonalization shell model code [7]. The main disadvantage of ANTOINE is that $J$ and $T$ are not good quantum numbers and the dimensions of the matrices are maximal.

One is then led to develop new tools to deal with the increasingly large model spaces needed in shell-model calculations. In this paper we present the first results obtained using a new code [NATHAN] [8,9], that works in $j$-$j$ coupling scheme and uses the quasi-spin formalism. This code retains the main idea of the code ANTOINE to calculate efficiently all non-zero matrix elements during the diagonalization procedure. It can be used either for unrestricted calculations as it is the case here, or for nuclei in which seniority truncations are physically sound as in the Sn region. The use of a $j$-$j$ coupling scheme allows us to reduce the the memory requirements with the penalty of an increase in CPU time. This increase is not so important as new computers double his speed every year and new shared-memory parallel machines are now available that allow for a relatively easy parallelization.

This paper has several goals: a) to report on results of the very large shell model calculations that can now be performed, b) to use them as benchmarks for the new approximate methods of solving the large scale shell model problem —e.g. Monte Carlo Shell Model [10] or Quantum Monte Carlo diagonalization method [11]— c) to analyze the systematics of binding energies for nuclei $40 \leq A \leq 56$, $20 \leq N, Z \leq 28$, extending the already published results for $A = 47$, 48 and 49 down to the beginning of the shell and up to the N=Z=28 closure, studying the effect of the scaling with the mass of the matrix elements. These three objectives will be dealt with in sections II, III and IV.

## II. THE SHELL MODEL CODE 'NATHAN'

For a long time, shell model calculations have been limited to ligth nuclei or to heavier ones with only a few particles outside closed shells. Besides the well known problems related to the determination of a good effective interaction for large valence spaces, there are compelling technical limitations due to the explosive increase of the dimensions of the matrices to diagonalize. The diagonalization in itself is not a problem since, in general, only a few eigenvectors are needed and in this case the Lanczos method is very efficient. For very large matrices, the convergence of the method is optimized by preliminary calculations in a truncated space. The fundamental problem is that we have to deal with "giant" matrices, giant meaning that the number of its non-zero elements is so large that it is impossible to store all of them before doing the Lanczos procedure. For this reason, one needs to compute all the non-zero terms at each new Lanczos iteration. It is clear that modern shell model codes must tackle this problem and that the quality of the code will be directly related to its performance in the calculation of non-zero terms during the Lanczos procedure itself.

The first breakthrough in this direction was due to the Glasgow group [12]. They took advantage of the simplicity of the m-scheme. In their code, each Slater determinant is represented by an integer word and each individual state by a bit in this word. Bit manipulation and bisection algorithms allow for a fast generation of the matrix elements. The shell model code ANTOINE adds some important improvements to the Glasgow method. The basic idea is to separate the total space in a product of the smaller spaces spanned by protons and neu-

trons. Then a state $I$ in the global basis can be labelled by a pair of proton($i$) and neutron ($\alpha$) states. All the $i(\alpha)$ states are classified in blocks defined by their $J_z$ value. To any proton block $J_z^p$ corresponds a neutron block $J_z^n = M - J_z^p$, where $M$ is the total angular momentum projection. Total wave functions are built by the association of a proton state $i$ (belonging to the block $J_z^p$) to a neutron state $\alpha$ (belonging to the corresponding block $J_z^n = M - J_z^p$). A simple numerical relation

$$I = R(i) + \alpha \tag{1}$$

can be established. Non-zero terms of the matrix are obtained through 3 integer additions: $I = R(i) + \alpha$, $J = R(j) + \beta$ and $H_{IJ} = V(K)$ with $K = Q(q) + \mu$. $q(\mu)$indices the one-body operator acting between $i(\alpha)$ and $j(\beta)$ states. $(i,j,q)$ and $(\alpha,\beta,\mu)$ are precalculated with the Glasgow method. The storage of these labels remains possible as the dimensions in respective proton and neutron spaces are moderated compared to those of the full space.

Another improvement that the code ANTOINE incorporates is an initial Lanczos procedure with the operators $J^2$ and $T^2$, i.e. a projection onto good $J$ and $T$. Basis states of good $J$ and $T$ are then used as initial states for the hamiltonian's Lanczos iterations. This accelerates the convergency dramatically.

The main disadvantage of the m-scheme is that the space comprises all the states with $J \geq J_z$ and $T \geq T_z$. The fundamental limitation is the capacity of storage the Lanczos vectors. For that reason, we have thought to adapt the idea of separating proton and neutron spaces to a coupled basis. Now, each $i$ and $\alpha$ functions are coupled to good angular momentum with the usual techniques of the Oak-Ridge/Rochester code [13]. The $i$ and $\alpha$ states are classified by their $J$ values. The fundamental difference with respect to the m-scheme is that now

- to a $J_p$ value correspond all the blocks $J_n$ with $|J_n - J_p| \leq J \leq J_n + J_p$.However, the relation $I = R(i) + \alpha$ remains valid.
- The N-body matrix elements are now given by the relation $H_{IJ} = h_{ij}.h_{\alpha\beta}.W(K)$, $h_{ij}(h_{\alpha\beta})$ being one-body matrix elements calculated with the Quasi-spin formalism and $W(K)$ being the product of a two-body matrix element with some $9j$ recoupling coeeficient. We notice that to the 3 previous additions to generate $H_{IJ}$ in the m-scheme case, we have to perform now 3 supplementary products.

To summarize, we can say that the two codes are complementary. The coupled formalism is more efficient in the following cases:

- For $J = 0^+$ states (the dimension is two orders of magnitude smaller than in the m-scheme) and to a lesser extent for low spin states.
- when we need a lot of Lanczos iterations(for the calculation of strength functions).
- When seniority truncations are reasonable.
- When the size of the m-scheme Lanczos vectors exceeds the storage capacity of the disks.

In other cases, the m-scheme code ANTOINE remains a better option. The two codes run on ordinary workstations. Indeed, the use of parallel computers should improve strongly their performances.

The code NATHAN has made it possible to carry out calculations that, if made in $m$-scheme, would involve more than one billion M=0 Slater determinants, as in our calculation of the ground state of $^{56}$Ni in the full $pf$-shell. The dimensions of the J=0 matrices together with their equivalent $m$-scheme dimensions are listed in table I for some of the nuclei we have studied in this work. Once the energy and the wave function of the ground state of a given nucleus is obtained, it is easy to built the doorway states (also named sum rule states) acting with the different transition operators $\Omega^\lambda$ on it. The norm of the doorway gives the non-energy weighted sum rule for the operator. If the doorway is used as starting vector in the Lanczos process, successive iterations provide the energy to the n-th weighted sum rules or equivalently the different moments of the strength function of the transition operator chosen. Notice that already with two iterations we have the norm, the centroid, the width and the skewness of the distribution of strength. These are averaged quantities that can also be accessed by the new stochastic approaches to the Shell Model problem, as for instance the Shell Model Monte Carlo (SMMC), and we shall devote the next section to compare the approximate and exact solutions.

## III. BENCHMARKS AND COMPARISON WITH SMMC RESULTS

With the advent of the stochastic approximations to the solution of the Shell Model problem, mentioned above, it becomes compulsory to dispose of large enough sets of exacts results in order to benchmark the accuracy of the new methods and to uncover their strong and weak aspects. We have chosen to make this comparison with the set of nuclei studied by Langanke *et al.* [14] using Caltech's SMMC. The effective interaction KB3 is used troughout, with effective charges 1.35 for protons and 0.35 for neutrons, bare $g$-factors and unquenched Gamow-Teller operator. The choice of an isoscalar effective charge of 1.7 in [14] instead of the canonical value of 2, leads to values that underpredict the experimental quadrupole transition rates. However this is irrelevant for our purpose of comparing SMMC and exact SM diagonalizations. SMMC involves two extrapolations; one in temperature and another in the parameter that has to be introduced [15] in order to change the sign of those terms of the hamiltonian that have "bad"-sign and that,

if taken at their original value, will spoil the convergence of the Monte Carlo method. Both extrapolations will contribute to the final differences with the exact results. While the defaults associated to the impossibility of doing a zero temperature calculation are smooth and predictable, those associated to the change of sign of the "bad"-sign terms are less well under control.

In table II we gather the energies and the E2 sum rules ($\sum_i B(E2)\ 0^+ \rightarrow 2_i^+$). SMMC gives energies that are above the exact values by about 0.5 MeV in most of the cases. This is consistent with a residual "heating" in SMMC. However, for the heaviest part of the set of nuclei studied, the discrepancies grow up to reach 2 MeV, indicating problems in the extrapolation linked to the "bad"-sign terms. The E2 sum rules are nicely reproduced by SMMC except in a couple of cases, $^{62}$Ni and $^{64}$Ni where the the exact number are clearly missed.

In table III the comparison is extended to M1 and Gamow-Teller sum rules. In most cases, the 10%–15% error bars of the SMMC numbers suffice to embrace the exact result. Nevertheless, there still remain some large deviations in the Gamow-Teller strength of $^{60}$Fe, $^{62}$Ni, $^{64}$Ni and $^{64}$Zn.

The outcome of this comparison is two-sided. On the one side, it validates SMMC to the 1–2 MeV level for the ground state energies and to the 20% level for the sum rules. On the other side, there are cases in which the discrepacies grow larger without an evident cause. This is a serious thread to the predictive power of SMMC, although it is envisageable that a more thorough control of the different extrapolations could bring these isolated cases to the general pace.

## IV. BINDING ENERGIES

The code NATHAN has given us the opportunity to complete our stock of binding energies of $pf$-shell nuclei, in the full space, using the effective interaction KB3. It is our aim now to verify that we can describe the ground state's energies at the same level of accuracy that we have achieved for the excitation energies ($\sim$ 200 keV). A remark is timely here; the monopole part of the interaction KB3 was fixed only by 1f7/2 nuclei, in a moment when only extremely truncated calculations were feasible. Therefore its non-1f7/2 monopoles are not well determined. Furthermore, its quasiparticle gap around $^{56}$Ni is too strong by about 1 MeV what will results in a relative underbinding of the nuclei with N or Z larger than 28. That is why in this section we shall only deal with 1f7/2 nuclei.

What the shell model calculation produces –E(SM) in the second column of table IV– is the contribution to the nuclear binding energy of the interaction of the valence particles among themselves. It does not include the Coulomb repulsion among the protons, nor the binding energy of the core ($^{40}$Ca in our case), nor the interaction among the core and the valence particles. Therefore, in order to compare with the experimental binding energies relative to $^{40}$Ca, $B_e$, we have take into account these quantities.

The Coulomb energies relative to $^{40}$Ca can be calculated using a local formula for a major shell ($\pi$ = valence protons, $\nu$ = valence neutrons):

$$E_C = e_\pi \pi + V_{\pi\pi} \frac{\pi(\pi-1)}{2} + V_{\pi\nu}\pi\nu. \qquad (2)$$

In our previous works [1,3] the values of the constants $e_\pi$, $V_{\pi\pi}$ and $V_{\pi\pi}$ were determined from the differences in binding energies between $^{41}$Sc and $^{40}$Ca ($e_\pi$) and the $A = 42$ isobars ($V_{\pi\pi}$ and $V_{\pi\nu}$). In this paper we are interested in larger mass region, hence the need of a better determination of the constants in expression (2). In order to do so we have fitted the Coulomb displacement energies of analog states for nuclei between $A = 42$ and $A = 64$ [16,17]. The resulting parameters are:

$$\begin{aligned} e_\pi &= 7.44 \pm 0.02, \\ V_{\pi\pi} &= 0.274 \pm 0.003, \\ V_{\pi\nu} &= -0.049 \pm 0.003. \end{aligned} \qquad (3)$$

Another option is to rely in global expressions that are used for the Coulomb term of the mass formulas. We have chosen the one used in ref [18];

$$E_C = 0.700(Z(Z-1) - 0.76(Z(Z-1))^{2/3})/R_C;$$
$$R_C = e^{\frac{1.5}{A}} \cdot A^{\frac{1}{3}} \cdot \left(0.946 - 0.573 \cdot \left(\frac{2T}{A}\right)^2\right) \qquad (4)$$

The valence space Coulomb energies obtained from (4) are very close to those from the local fit (2), with discrepancies that never reach 1%. In what follows we shall use the Coulomb energies from the global formula (4).

Besides, one should add the nuclear interaction between a particle in the valence space and the core. The value of this –one body– matrix element is usually taken from the binding energy difference between $^{41}$Ca and $^{40}$Ca. However we shall proceed otherwise; as the effective interaction we have been using (KB3), has been only tested against spectroscopic observables that will not vary if we add to the hamiltonian terms that only depend on scalars made with the **total** number of valence particles (n) or the **total** isospin (T), we have the freedom to add the following monopole expression to our hamiltonian:

$$E_M = e_v\ n + a\ \frac{1}{2} n(n-1) + b\ (T(T+1) - \frac{3}{4}\ n) \qquad (5)$$

where $e_v$ is an average particle core interaction (hopefully close to the one experimentally determined in A=41) and a and b are the isoscalar and isovector global monopole corrections to KB3 that we will fix by a fit to the experimental binding energies relative to $^{40}$Ca using the formula:

$$E_B = -B_e = E(SM) + E_C + E_M, \qquad (6)$$

The data set is listed in the fourth column of table IV (the numbers with a star are extrapolated values from [19] not included in the fit) and contains 51 entries. The values of the parameters resulting from the fit are:

$$\begin{aligned} e_v &= -8.67 \pm 0.01\ MeV, \\ a &= 0.092 \pm 0.003\ MeV, \\ b &= 0.063 \pm 0.006\ MeV. \end{aligned}$$

The Shell Model binding energies calculated with these values are listed in the third column of table IV. The rms deviation between theory and experiment is 227 keV. These results deserve some comments:

– The rms deviation we have attained fulfils our expectations; we are able to describe consistently at the same level of accuracy excitation energies and –valence space– ground state energies.

– The value $e_v$=-8.67 MeV is close enough to the A=41 value -8.36 MeV as to be considered satisfactory.

– The values of the a and b parameters are small and indeed smaller than the monopole modifications of some terms of the original Kuo-Brown interaction that led to KB3 (about 300 keV).

– The Shell Model binding energies for those nuclei not included in the fit are our barest predictions. If we compare them with the extrapolated values in [19] the discrepancies are somewhat larger than for the measured values, without exceeding 500 keV in any case.

There are basic reasons to scale the matrix elements of the effective interactions with a term that reflects somehow the change in size of the underlying mean field. In the harmonic oscillator basis this brings in the usual $A^{1/3}$ dependence of $\hbar\omega$, that has been sometimes incorporated to $sd$ and $pf$-shell effective interactions [20–22]. A more elaborated dependence has been proposed recently [23] in order to improve the description of nuclear radii. It leads to the following scaling factor:

$$\left(\frac{A_0}{A}\right)^{\frac{1}{3}} \cdot e^{3\left(\frac{A-A_0}{A\cdot A_0}\right)} \cdot \left(\frac{0.946 - 0.573\left(\frac{2T}{A_0}\right)^2}{0.946 - 0.573\left(\frac{2T}{A}\right)^2}\right)^2 \qquad (7)$$

where $A_0$ is the mass at which the effective interaction has been computed and A and T are the mass and the isospin of the nucleus we are dealing with.

It is worth noticing that the lower $pf$-shell might be special in which has to do with global scalings, because the radii of $^{40}$Ca and $^{58}$Ni can be reproduced without any change in the harmonic oscillator size parameter and so do the Coulomb displacement energies [24]. On the other side we wondered whether the extra global monopole correction that comes out of our fit is an artefact due precisely to the absence of mass dependence in the matrix elements or not. In order to settle this point we have repeated all the binding energy calculations with matrix elements scaled as in equation (7) with $A_0$=42 (see table V). Afterwords, we follow exactly the same steps discussed above; we add the same Coulomb energies and proceed to fit the coefficients of the global monopole formula (5), but now with the a and b parameters scaling as the matrix elements. The values of the parameters at A=42 are:

$$\begin{aligned} e_v &= -8.61 \pm 0.01\ MeV, \\ a &= 0.041 \pm 0.003\ MeV, \\ b &= 0.119 \pm 0.006\ MeV. \end{aligned}$$

The resulting binding energies are compared in table V with the experimental data. The rms deviation is now 215 keV. Therefore we are led to conclude that the average quality of the agreement is insensitive to the inclusion of a mass dependence in the two body matrix elements. Notice that the value of $e_v$ is essentially the same we had without mass dependence. On the other hand the a and b parameters are quite different from the ones we had, even if they are in the same range of values. It appears that one half of the global isoscalar monopole correction can be absorbed into the mass dependence, on the contrary the isovector correction doubles. The predictions for the binding energies not included in the fit differ from those of the previous one typically by 150 keV, in the direction of increasing the discrepancy with the extrapolated values. Nevertheles none of this elements is decisive in making a choice between the two approaches. On the one side, Occam's razor favours the mass independent choice, on the other side, if we want to go beyond $^{56}$Ni we should surely need to incorporate the mass dependence.

## V. CONCLUSIONS

The new shell model code NATHAN has been used to calculate the binding energies, M1, E2 and GT sum rules of several nuclei nuclei of the $pf$-shell, in the full valence space, using the effective interction KB3. These results have been used to benchmark the SMMC calculations, that agree with the exact results within 20% in most cases. We have also computed the binding energy of nearly all $1f_{7/2}$ nuclei, reaching the same level of agreement than we had for the excitation energies and making predictions for a number of still unavailable masses. We also show that the inclusion of a mass dependence in the two body matrix elements is not critical for the description of the binding energies in this region.

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[1] E. Caurier, A. P. Zuker, A. Poves, and G. Martínez-Pinedo, Phys. Rev. C**50** (1994) 225.

[2] E. Caurier, J. L. Egido, G. Martínez-Pinedo, A. Poves, J. Retamosa, L. M. Robledo and A. P. Zuker, Phys. Rev. Lett. **75** (1995) 2466.

[3] G. Martínez-Pinedo, A. P. Zuker, A. Poves and E. Caurier, Phys. Rev. C **55** (1997) 187.

[4] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **A114** (1968) 241.

[5] A. Poves and A. P. Zuker, Phys. Rep. **70** (1990) 235.

[6] E. Caurier, computer code ANTOINE, CRN, Strasbourg (1989).

[7] C. Ur et al., Phys. Rev. C (in press).

[8] F. Nowacki, E. Caurier, coupled code NATHAN, Strasbourg (1995).

[9] F. Nowacki, Ph. D. thesis (Strasbourg, 1996).

[10] S. E. Koonin, D. J. Dean and K. Langanke, Phys. Rep. **278** (1997) 1.

[11] M. Honma, T. Mizusaki, T. Otsuka, Phys. Rev. Lett. **77** (1996) 3315.

[12] R. R. Whitehead, A. Watt, B. J. Cole and I. Morrison Adv. in Nuc. Phys. vol. 9 (1977) 123.

[13] J. B. French, E. C. Halbert, J. B. McGrory and S. S. M. Wong, Adv. in Nuc. Phys. vol. 3 (1969) 237.

[14] K. Langanke, D. J. Dean, P. B. Radha, Y. Alhassid and S. E. Koonin, Phys. Rev. C **52** (1995) 718.

[15] Y. Alhassid, D. J. Dean, S. E. Koonin, G. Lang and W. E. Ormand, Phys. Rev. Lett. **72** (1994) 613.

[16] M. S. Anthony, J. Britz, J. B. Bueb and A. Pape, At. Data Nucl. Data Tables **33**, 448 (1985).

[17] M. S. Anthony, J. Britz, and A. Pape, At. Data Nucl. Data Tables **40**, 10 (1988).

[18] J. Duflo and A. Zuker, Phys. Rev. C **52** (1995) R23.

[19] G. Audi and A. H. Wapstra, Nucl. Phys. **A595** (1995) 409.

[20] B. H. Wildenthal Prog. Part. Nucl. Phys. **11** (1984) 5.

[21] W. A. Richter, M. G. Van der Merwe, R. E. Julies and B. A. Brown, Nucl. Phys. **A523** (1991) 325.

[22] J. Retamosa, E. Caurier, F. Nowacki and A. Poves, Phys. Rev. C **55** (1997) 1255.

[23] J. Duflo and A. Zuker, private communication.

[24] J. M. Gomez, Phys. Lett. **B62** (1976) 25.


TABLE I. $m$ scheme and $J = 0$ dimensions in the full $pf$ shell

| Nucleus | $m$ scheme | $J = 0$ dimension |
|---|---|---|
| $^{48}$Ti | 634 744 | 14 177 |
| $^{50}$Ti | 1 967 848 | 39 899 |
| $^{52}$Ti | 2 843 770 | 55 944 |
| $^{50}$Cr | 14 625 240 | 267 054 |
| $^{52}$Cr | 45 734 928 | 773 549 |
| $^{54}$Cr | 66 262 352 | 1 093 850 |
| $^{52}$Fe | 109 954 620 | 1 777 116 |
| $^{54}$Fe | 345 400 174 | 5 220 621 |
| $^{56}$Fe | 501 113 392 | 7 413 488 |
| $^{56}$Ni | 1 087 455 228 | 15 443 684 |

TABLE II. Valence energies and B(E2) sum rules, exact diagonalization vs. Shell Model Monte Carlo results

| nucleus | $E(SM)$ (shell model) | $E(SM)$ (SMMC) | $\sum B(E2)$ (shell model) | $\sum B(E2)$ (SMMC) |
|---|---|---|---|---|
| $^{48}$Ti | −24.6 | −23.9 | 476 | 455 ± 25 |
| $^{50}$Ti | −27.7 | −27.2 | 405 | 465 ± 50 |
| $^{52}$Ti | −25.4 | −24.9 | 477 | 465 ± 55 |
| $^{54}$Ti | −22.0 | −21.4 | 445 | 450 ± 80 |
| $^{48}$Cr | −32.9 | −32.3 | 978 | 945 ± 45 |
| $^{50}$Cr | −40.5 | −40.0 | 913 | 890 ± 90 |
| $^{52}$Cr | −46.0 | −45.6 | 690 | 645 ± 75 |
| $^{54}$Cr | −47.0 | −46.3 | 888 | 890 ± 90 |
| $^{56}$Cr | −45.5 | −44.8 | 825 | 840 ± 90 |
| $^{52}$Fe | −54.3 | −53.7 | 1016 | 1055 ± 50 |
| $^{54}$Fe | −62.8 | −62.7 | 764 | 750 ± 80 |
| $^{56}$Fe | −66.4 | −65.8 | 1019 | 990 ± 6 |
| $^{58}$Fe | −67.7 | −66.7 | 1117 | 1010 ± 65 |
| $^{60}$Fe | −67.0 | −65.8 | 1052 | 1105 ± 65 |
| $^{56}$Ni | −78.5 | −77.8 | 572 | 515 ± 65 |
| $^{62}$Ni | −89.5 | −87.6 | 823 | 1010 ± 25 |
| $^{64}$Ni | −89.9 | −87.7 | 773 | 1165 ± 80 |
| $^{64}$Zn | −106.3 | −104.8 | 1157 | 1225 ± 65 |

TABLE III. 1 and Gamow-Teller sum rules, exact diagonalization vs. Shell Model Monte Carlo results

| Nucleus | $\sum B(M1)$ (shell model) | $\sum B(M1)$ (SMMC) | $\sum B(GT_+)$ (shell model) | $\sum B(GT_+)$ (SMMC) |
|---|---|---|---|---|
| $^{48}$Ti | 10.6 | 10.2 ± 1.2 | 1.26 | 1.13 ± 0.18 |
| $^{50}$Ti | 12.6 | 12.5 ± 1.0 | 1.24 | 1.47 ± 0.16 |
| $^{52}$Ti | 12.9 | 12.5 ± 1.0 | 0.99 | 1.11 ± 0.16 |
| $^{54}$Ti | 13.4 | 13.5 ± 1.5 | 0.89 | 0.97 ± 0.21 |
| $^{48}$Cr | 12.0 | 13.8 ± 1.7 | 4.13 | 4.37 ± 0.35 |
| $^{50}$Cr | 13.9 | 14.5 ± 2.5 | 3.57 | 3.51 ± 0.27 |
| $^{52}$Cr | 15.6 | 18.9 ± 2.2 | 3.33 | 3.51 ± 0.19 |
| $^{54}$Cr | 16.5 | 13.0 ± 2.5 | 2.24 | 2.21 ± 0.22 |
| $^{56}$Cr | 16.3 | 16.2 ± 2.0 | 1.92 | 1.50 ± 0.21 |
| $^{52}$Fe | 17.2 | 18.9 ± 1.4 | 6.92 | 7.10 ± 0.42 |
| $^{54}$Fe | 18.9 | 16.5 ± 2.8 | 6.33 | 6.05 ± 0.45 |
| $^{56}$Fe | 19.4 | 20.4 ± 3.0 | 4.69 | 3.99 ± 0.27 |
| $^{58}$Fe | 18.8 | 20.3 ± 3.0 | 3.12 | 3.06 ± 0.28 |
| $^{60}$Fe | 18.2 | 17.3 ± 2.1 | 2.60 | 1.80 ± 0.24 |
| $^{56}$Ni | 22.8 | 23.0 ± 1.2 | 10.2 | 9.86 ± 0.38 |
| $^{62}$Ni | 20.7 | 19.6 ± 2.9 | 4.38 | 3.43 ± 0.40 |
| $^{64}$Ni | 19.3 | 18.9 ± 2.7 | 3.44 | 1.73 ± 0.29 |
| $^{64}$Zn | 21.6 | 23.6 ± 2.2 | 5.54 | 4.13 ± 0.34 |

TABLE IV. Shell model binding energies relative to $^{40}$Ca compared with experiment. KB3 interaction without mass dependence, see text for the details

| Nucleus | $E(SM)$ | $B_e$(th) | $B_e$(exp) | $\Delta$ |
|---|---|---|---|---|
| $^{42}$Ca | −2.71 | 19.93 | 19.84 | 0.08 |
| $^{42}$Sc$^{T=1}$ | −2.71 | 12.44 | 12.64 | −0.20 |
| $^{42}$Sc$^{T=0}$ | −2.35 | 12.20 | 12.02 | 0.17 |
| $^{42}$Ti | −2.71 | 4.55 | 4.85 | −0.30 |
| $^{43}$Ca | −2.55 | 28.19 | 27.78 | 0.41 |
| $^{43}$Sc | −6.67 | 25.06 | 24.77 | 0.29 |
| $^{43}$Ti | −6.67 | 17.24 | 17.12 | 0.12 |
| $^{43}$V | −2.55 | 4.72 | 5.05* | −0.32 |
| $^{44}$Ca | −4.99 | 38.93 | 38.91 | 0.02 |
| $^{44}$Sc | −8.26 | 35.07 | 34.47 | 0.60 |
| $^{44}$Ti | −13.88 | 33.06 | 33.42 | −0.37 |
| $^{44}$V | −8.26 | 19.16 | 18.94* | 0.22 |
| $^{44}$Cr | −4.99 | 7.11 | 7.84* | −0.74 |
| $^{45}$Ca | −4.61 | 46.73 | 46.32 | 0.41 |
| $^{45}$Sc | −10.95 | 46.06 | 45.80 | 0.27 |
| $^{45}$Ti | −15.49 | 43.09 | 42.95 | 0.14 |
| $^{45}$V | −15.49 | 35.00 | 35.04 | −0.04 |
| $^{45}$Cr | −10.95 | 21.80 | 21.79* | 0.00 |
| $^{45}$Mn | −4.61 | 6.28 | 6.71* | −0.43 |
| $^{46}$Ca | −6.73 | 56.90 | 56.72 | 0.18 |
| $^{46}$Sc | −11.67 | 54.94 | 54.56 | 0.39 |
| $^{46}$Ti | −20.14 | 56.02 | 56.14 | −0.12 |
| $^{46}$V$^{T=1}$ | −20.14 | 47.99 | 48.31 | −0.32 |
| $^{46}$V$^{T=0}$ | −19.77 | 47.75 | 47.51 | 0.24 |
| $^{46}$Cr | −20.14 | 39.58 | 39.92 | −0.35 |
| $^{46}$Mn | −11.67 | 22.06 | 22.04* | 0.02 |
| $^{46}$Fe | −6.73 | 7.57 | 8.13* | −0.56 |
| $^{47}$Ca | −6.10 | 64.20 | 63.99 | 0.21 |
| $^{47}$Sc | −14.05 | 65.37 | 65.20 | 0.17 |
| $^{47}$Ti | −21.06 | 65.11 | 65.02 | 0.09 |
| $^{47}$V | −25.07 | 61.33 | 61.31 | 0.02 |
| $^{47}$Cr | −25.07 | 52.98 | 53.08 | −0.10 |
| $^{47}$Mn | −21.06 | 40.05 | 40.00* | 0.05 |
| $^{47}$Fe | −14.05 | 23.61 | 23.58* | 0.03 |
| $^{48}$Ca | −7.88 | 73.79 | 73.94 | −0.15 |
| $^{48}$Sc | −14.13 | 73.37 | 73.43 | −0.07 |
| $^{48}$Ti | −24.57 | 76.65 | 76.65 | 0.00 |
| $^{48}$V | −27.58 | 71.99 | 71.85 | 0.14 |
| $^{48}$Cr | −32.95 | 69.20 | 69.41 | −0.21 |
| $^{48}$Mn | −27.58 | 55.03 | 54.81* | 0.22 |
| $^{48}$Fe | −24.57 | 42.72 | 43.14* | −0.42 |
| $^{48}$Co | −14.13 | 22.48 | 22.61* | −0.13 |
| $^{49}$Sc | −16.19 | 83.23 | 83.57 | −0.34 |
| $^{49}$Ti | −24.81 | 84.80 | 84.79 | 0.01 |
| $^{49}$V | −31.01 | 83.45 | 83.40 | 0.04 |
| $^{49}$Cr | −35.59 | 79.98 | 79.99 | −0.01 |
| $^{49}$Mn | −35.59 | 71.37 | 71.49 | −0.13 |
| $^{49}$Fe | −31.01 | 57.61 | 57.68* | −0.07 |
| $^{49}$Co | −24.81 | 41.74 | 41.90* | −0.15 |
| $^{50}$Ti | −27.72 | 95.49 | 95.73 | −0.24 |
| $^{50}$V | −32.16 | 92.50 | 92.74 | −0.24 |
| $^{50}$Cr | −40.54 | 92.95 | 92.99 | −0.05 |
| $^{50}$Mn$^{T=1}$ | −40.54 | 84.39 | 84.58 | −0.18 |
| $^{50}$Mn$^{T=0}$ | −40.28 | 84.26 | 84.35 | −0.09 |
| $^{50}$Fe | −40.54 | 75.47 | 75.64 | −0.18 |
| $^{50}$Co | −32.16 | 57.55 | 57.59* | −0.04 |
| $^{50}$Ni | −27.72 | 43.06 | 43.40* | −0.34 |
| $^{51}$V | −35.31 | 103.42 | 103.79 | −0.37 |
| $^{51}$Cr | −41.81 | 102.10 | 102.25 | −0.15 |
| $^{51}$Mn | −46.17 | 98.16 | 98.26 | −0.11 |
| $^{51}$Fe | −46.17 | 89.29 | 89.46 | −0.17 |
| $^{51}$Co | −41.81 | 75.51 | 75.74* | −0.23 |
| $^{51}$Ni | −35.31 | 59.09 | 59.12* | −0.03 |
| $^{52}$Cr | −45.99 | 114.05 | 114.29 | −0.24 |
| $^{52}$Fe | −54.27 | 105.46 | 105.64 | −0.19 |
| $^{52}$Ni | −45.99 | 78.08 | 78.41* | −0.32 |
| $^{54}$Fe | −62.85 | 129.63 | 129.71 | −0.07 |
| $^{54}$Co | −62.85 | 120.57 | 120.68 | −0.11 |
| $^{54}$Ni | −62.85 | 111.15 | 111.10 | 0.05 |
| $^{56}$Ni | −78.46 | 142.44 | 141.94 | 0.50 |

TABLE V. Shell model binding energies relative to $^{40}$Ca compared with experiment. KB3 interaction with mass dependence, see text for the details

| Nucleus | $E(SM)$ | $B_e$(The) | $B_e$(Exp) | $\Delta$ |
|---|---|---|---|---|
| $^{42}$Ca | −2.71 | 19.83 | 19.84 | −0.01 |
| $^{42}$Sc$^{T=1}$ | −2.71 | 12.34 | 12.64 | −0.30 |
| $^{42}$Sc$^{T=0}$ | −2.35 | 12.21 | 12.02 | 0.19 |
| $^{42}$Ti | −2.71 | 4.45 | 4.85 | −0.40 |
| $^{43}$Ca | −2.53 | 28.06 | 27.78 | 0.28 |
| $^{43}$Sc | −6.62 | 25.07 | 24.77 | 0.30 |
| $^{43}$Ti | −6.62 | 17.25 | 17.12 | 0.12 |
| $^{43}$V | −2.53 | 4.59 | 5.05* | −0.45 |
| $^{44}$Ca | −4.92 | 38.76 | 38.91 | −0.14 |
| $^{44}$Sc | −8.14 | 35.08 | 34.47 | 0.60 |
| $^{44}$Ti | −13.67 | 33.08 | 33.42 | −0.34 |
| $^{44}$V | −8.14 | 19.16 | 18.94* | 0.23 |
| $^{44}$Cr | −4.92 | 6.94 | 7.84* | −0.90 |
| $^{45}$Ca | −4.51 | 46.58 | 46.32 | 0.25 |
| $^{45}$Sc | −10.72 | 46.05 | 45.80 | 0.25 |
| $^{45}$Ti | −15.16 | 43.13 | 42.95 | 0.18 |
| $^{45}$V | −15.16 | 35.05 | 35.04 | 0.01 |
| $^{45}$Cr | −10.72 | 21.78 | 21.79* | −0.01 |
| $^{45}$Mn | −4.51 | 6.13 | 6.71* | −0.58 |
| $^{46}$Ca | −6.54 | 56.73 | 56.72 | 0.02 |
| $^{46}$Sc | −11.35 | 54.97 | 54.56 | 0.41 |
| $^{46}$Ti | −19.57 | 56.01 | 56.14 | −0.13 |
| $^{46}$V$^{T=1}$ | −19.57 | 47.98 | 48.31 | −0.33 |
| $^{46}$V$^{T=0}$ | −19.21 | 47.85 | 47.51 | 0.35 |
| $^{46}$Cr | −19.57 | 39.57 | 39.92 | −0.36 |
| $^{46}$Mn | −11.35 | 22.09 | 22.04* | 0.05 |
| $^{46}$Fe | −6.54 | 7.41 | 8.13* | −0.73 |
| $^{47}$Ca | −5.90 | 64.12 | 63.99 | 0.13 |
| $^{47}$Sc | −13.58 | 65.39 | 65.20 | 0.19 |
| $^{47}$Ti | −20.36 | 65.16 | 65.02 | 0.14 |
| $^{47}$V | −24.20 | 61.38 | 61.31 | 0.07 |
| $^{47}$Cr | −24.20 | 53.03 | 53.08 | −0.05 |
| $^{47}$Mn | −20.36 | 40.10 | 40.00* | 0.10 |
| $^{47}$Fe | −13.58 | 23.64 | 23.58* | 0.05 |
| $^{48}$Ca | −7.58 | 73.74 | 73.94 | −0.20 |
| $^{48}$Sc | −13.59 | 73.50 | 73.43 | 0.07 |
| $^{48}$Ti | −23.60 | 76.66 | 76.65 | 0.02 |
| $^{48}$V | −26.49 | 72.10 | 71.85 | 0.25 |
| $^{48}$Cr | −31.61 | 69.16 | 69.41 | −0.25 |
| $^{48}$Mn | −26.49 | 55.14 | 54.81* | 0.33 |
| $^{48}$Fe | −23.60 | 42.74 | 43.14* | −0.40 |
| $^{48}$Co | −13.59 | 22.61 | 22.61* | 0.00 |
| $^{49}$Sc | −15.48 | 83.41 | 83.57 | −0.16 |
| $^{49}$Ti | −23.70 | 84.95 | 84.79 | 0.16 |
| $^{49}$V | −29.61 | 83.56 | 83.40 | 0.16 |
| $^{49}$Cr | −33.96 | 80.02 | 79.99 | 0.03 |
| $^{49}$Mn | −33.96 | 71.41 | 71.49 | −0.08 |
| $^{49}$Fe | −29.61 | 57.73 | 57.68* | 0.05 |
| $^{49}$Co | −23.70 | 41.89 | 41.90* | 0.00 |
| $^{50}$Ti | −26.34 | 95.66 | 95.73 | −0.07 |
| $^{50}$V | −30.57 | 92.76 | 92.74 | 0.02 |
| $^{50}$Cr | −38.47 | 92.94 | 92.99 | −0.05 |
| $^{50}$Mn$^{T=1}$ | −38.47 | 84.39 | 84.58 | −0.19 |
| $^{50}$Mn$^{T=0}$ | −38.25 | 84.39 | 84.35 | 0.04 |
| $^{50}$Fe | −38.47 | 75.46 | 75.64 | −0.18 |
| $^{50}$Co | −30.57 | 57.80 | 57.59* | 0.22 |
| $^{50}$Ni | −26.34 | 43.23 | 43.40* | −0.17 |
| $^{51}$V | −33.37 | 103.71 | 103.79 | −0.07 |
| $^{51}$Cr | −39.49 | 102.27 | 102.25 | 0.02 |
| $^{51}$Mn | −43.60 | 98.22 | 98.26 | −0.04 |
| $^{51}$Fe | −43.60 | 89.35 | 89.46 | −0.11 |
| $^{51}$Co | −39.49 | 75.68 | 75.74* | −0.06 |
| $^{51}$Ni | −33.37 | 59.38 | 59.12* | 0.27 |
| $^{52}$Cr | −43.21 | 114.21 | 114.29 | −0.08 |
| $^{52}$Fe | −50.95 | 105.38 | 105.64 | −0.27 |
| $^{52}$Ni | −43.21 | 78.24 | 78.41* | −0.16 |
| $^{54}$Fe | −58.46 | 129.70 | 129.71 | −0.01 |
| $^{54}$Co | −58.46 | 120.63 | 120.68 | −0.05 |
| $^{54}$Ni | −58.46 | 111.21 | 111.10 | 0.11 |
| $^{56}$Ni | −72.31 | 142.38 | 141.94 | 0.44 |